Polaronic effect on the electron energy spectrum in a quantum well

1994 J. Phys.: Condens. Matter 6 10307

(http://iopscience.iop.org/0953-8984/6/47/014)

J. Phys.: Condens. Matter 6 (1994) 10307–10316. Printed in the UK

Polaronic effect on the electron energy spectrum in a quantum well

Ruisheng Zheng†, Shiliang Ban†‡ and Xi Xia Liang†‡

† Department of Physics, Inner Mongolia University, Hohhot 010021, People's Republic of China

‡ Chinese Center of Advanced Science and Technology (World Laboratory), PO Box 8730, Beijing 100080, People's Republic of China

Received 25 May 1994, in final form 17 July 1994

Abstract. A general analytical expression for the electron energy spectrum and the polaron binding energy for different electronic subband bound states in a quantum well (QW) is presented. The effects of the electron–optical-phonon interaction, the finite confinement potential, the difference in the electronic effective masses across the interface, and the electron subband state are considered in this paper. The correct three-dimensional and two-dimensional results are given as the limit cases when the well width varies from infinity to zero. The expression is numerically applied to the GaAs/$Al_xGa_{1-x}As$ QWs with several different aluminium concentrations x. Some properties of the polaron are discussed.

1. Introduction

The property of a polaron confined in a quantum well (QW) has been a topic of considerable interest in recent years. The QW structure is a low-dimensional layered structure and is frequently fabricated from weakly ionic semiconductors (the GaAs/$Al_xGa_{1-x}As$ case is a typical example) and therefore the interaction of the electron with polar-optical phonons is in general important for the determination of electron dynamics in such structures. Most of the early work treated the polaronic effect in QW structure by considering that the electron has a quasi-two-dimensional (Q2D) character and the phonons have a three-dimensional (3D) character regardless of the influence of the interfaces of the system on the phonons, and especially on the long-wavelength longitudinal optical (LO) phonons. This was considered to be plausible because of the small differences in the mechanical and electrical properties throughout the QW. Using this approximation, many researchers [1–5] studied the properties of the electron–phonon interaction system in a QW and obtained many useful results. However, after some fundamental investigations by several groups [6–14], it is clear that the real situation is rather different. The polar-optical phonons in a layered structure behave as in a confined system; its penetration from a given layer into the adjacent layers is really inhibited owing to rather different vibration frequencies in the layers. There are three types of optical phonon mode which should be considered in a reliable polaron theory for use in the QW case:

(1) the four branches of interface optical (IO) phonon modes;
(2) the confined slab LO mode in the well;
(3) the half-space LO mode in the barrier.

0953-8984/94/4710307+10$19.50

On the basis of the considerations mentioned above, some more accurate theories for polarons in QWs have been proposed recently. Using the second-order perturbation method, some workers [15, 16] studied the properties of the Q2D polaron. It was soon realized that it is necessary to incorporate all the energy states as intermediate states in the calculation; otherwise it is impossible to obtain the correct result. More recently, Hai *et al* [17] improved their work by incorporating the full subband energy spectrum as intermediate states in their second-order perturbation calculation. After a tedious analytical and numerical calculation, they gave a better numerical result for the binding energy and effective mass which has correct limit approaches for a polaron in a $GaAs/Al_xGa_{1-x}As$ QW.

More recently, the present authors [18, 19] have proposed a variational calculation method for treating the quasi-low-dimensional electron–phonon interaction system. This method is simple but very effective. The main advantage of our method is that an analytical expression for the binding energy of the Q2D polaron can be obtained, in which the transition from the 2D to the 3D limit is correctly obtained. From the analytical expression the relative importance of every phonon mode as a function of the well width, the well potential height and the concentration of the compounds is clearly shown.

The purpose of the present paper is to report a more advanced investigation of the properties of a Q2D polaron in a QW. All the possible electron–optical-phonon interactions in the QW structure, the effects of the finite electronic confinement potential, the electronic subband states, and the electron band mass difference on the two sides of the interfaces are considered in this paper. An improved theoretical result for the polaron binding energy with different electronic subband states of the Q2D electron is presented analytically. In the limits of infinitely wide and infinitely narrow wells, our expression gives the correct 3D and 2D results, respectively. In the infinite QW approximation or same-electron-band-mass approximation, the expression agrees with our previous papers. The expression is numerically applied to $GaAs/Al_xGa_{1-x}As$ QWs with several different aluminium concentrations x. The contributions and the relative importance of the IO-, confined LO- and half-space LO-phonon modes to the polaron corrections are shown clearly as the well width is varied from infinity to zero.

The paper is organized as follows: in section 2, first, we give a short review of the Hamiltonian, next the variational calculation is presented, and then the analytical result for the bound-state energy and the polaron binding energy of the Q2D electron–phonon interaction system is given. The numerical results for $GaAs/Ga_{1-x}Al_xAs$ QWs (with $x = 0.3$ and 1.0) are also shown graphically in section 2. A discussion and the conclusion are given in section 3.

2. Calculation and results

The Hamiltonian of an electron interacting with optical phonons in a finite deep QW made up of two different polar semiconductors has been described in our previous paper [19]. In the present paper a more accurate Hamiltonian model is considered by including the difference in the electron effective masses across the interface. Here we give a short review of it for completeness. The Hamiltonian has seven parts and is written

$$H = H_e + H_{IO} + H_{e-IO} + H_{LO} + H_{e-LO1} + H_{LO2} + H_{e-LO2}. \tag{1}$$

It is a sum of the Hamiltonians of, in the order given above, the bare confined electron, the free IO phonon, the electron–IO-phonon interaction, the free confined LO phonon in the

well material, the electron-confined LO–phonon interaction, the free half-space LO phonon in the barrier material, and the electron–half-space LO-phonon interaction. The Hamiltonian is taken from the fundamental work in [6, 10].

In this paper the effective band mass and rectangular QW approximation are used; the electron band mass and the QW confinement potential are taken as

$$m_b = \begin{cases} m_{b1} & |z| > d \\ m_{b2} & |z| \leqslant d \end{cases} \tag{2}$$

$$V(z) = \begin{cases} V_0 & |z| > d \\ 0 & |z| \leqslant d \end{cases} \tag{3}$$

where m_{b1} (m_{b2}) is the electron band mass in the well (barrier) material. $W = 2d$ is the width of the QW.

The above Hamiltonian is so complicated that accurate solutions of the eigenfunction and eigenvalue are impossible; therefore some approximation method must be used. We adopt a variational method which has been proposed in our previous paper [19]. The trial wavefunction $|\psi\rangle$ of the Hamiltonian is chosen as

$$|\psi\rangle = U|0\rangle|\Phi_l\rangle \tag{4}$$

where $|\Phi_l\rangle$ is the eigenstate of the Hamiltonian H_e. Here we are only interested in the bound state of the confined electron and assume that the momentum of the electron in the x–y plane is zero. Therefore, the eigenfunction Φ_l is the function of the z component only. $|0\rangle$ is the phonon vacuum state. U is a unitary transformation operator, which is given by

$$U = \exp\left(\sum_{k,m}[F_{km}(z)\exp(-i\boldsymbol{k}\cdot\rho)a^+_{km} - \text{HC}) + \sum_{k,k_z}(Q_{k,k_z}(z)\exp(-i\boldsymbol{k}\cdot\rho)a^+_{k,k_z} - \text{HC}) + \sum_{k,\sigma,p}(G_{k\sigma p}(z)\exp(-i\boldsymbol{k}\cdot\rho)a^+_{k\sigma p} - \text{HC})\right) \tag{5}$$

in which

$$F_{km}(z) = f_{km}\sin[k_m(z+d)]\theta(d-|z|) \tag{6}$$

$$Q_{k,k_z}(z) = q_{k,k_z}\sin[k_z(|z|-d)]\theta(|z|-d) \tag{7}$$

$$G_{k\sigma p}(z) = g_{k\sigma p}L_{k\sigma p}(z) \tag{8}$$

where f_{km}, q_{k,k_z} and $g_{k\sigma p}$ are the variational parameters which will be subsequently determined by standard variational calculations.

$\Phi_l(z)$ is the eigenfunction of the bare confined electron described by the Hamiltonian H_e, which is either even or odd in the z direction and given by

$$\Phi_l^{(e)}(z) = \begin{cases} N_l\cos(k_l d)\exp[-k'_l(|z|-d)] & |z| > d \\ N_l\cos(k_l z) & |z| \leqslant d \end{cases} \qquad l = 1, 3, 5, \ldots \tag{9}$$

$$\Phi_l^{(0)}(z) = \begin{cases} \text{sgn}(z)N_l\sin(k_l d)\exp[-k'_l(|z|-d)] & |z| > d \\ N_l\sin(k_l z) & |z| \leqslant d \end{cases} \qquad l = 2, 4, 6, \ldots \tag{10}$$

where the wavenumbers k_l and k_l' are related to the electron subband energy E_l by

$$k_l = \sqrt{\frac{2m_{b1}E_l}{\hbar^2}} \qquad k_l' = \sqrt{\frac{2m_{b2}(V_0 - E_l)}{\hbar^2}}. \tag{11}$$

The form of the normalization constant N_l depends on the condition determining the eigenstate. According to Bastard's [20] work, the corresponding bound-state equations are determined by the boundary conditions that $\Phi_l(z)$ and $m_b^{-1}(\partial\Phi_l/\partial z)$ are both continuous at the interfaces ($z = \pm d$). The electron subband energy E_l can be determined from the boundary conditions. Because this is a standard quantum mechanics textbook problem and the calculation details are well known, there is no need to repeat them here. Then N_l can be expressed as a function of the electron subband energy E_l only:

$$N_l = \left(d + \frac{C_l}{k_l} + \frac{D_l}{k_l'}\right)^{-1/2} \tag{12}$$

with

$$C_l = \left[\frac{m_{b1}}{m_{b2}}\left(\frac{V_0}{E_l} - 1\right) + 1\right]^{-1} \tag{13}$$

$$D_l = \left[\frac{m_{b1}}{m_{b2}}\left(\frac{V_0}{E_l} - 1\right)\right]^{1/2} C_l. \tag{14}$$

The expectation value of the Hamiltonian of the Q2D polaron system is

$$E = \langle\psi|H|\psi\rangle = \langle\Phi_l|\langle 0|U^+HU|0\rangle|\Phi_l\rangle. \tag{15}$$

After lengthy variational calculation, we finally obtain the expression for the energy spectrum E of the Q2D electron–phonon interaction system in any electronic subband state, which is given by

$$E = E_l - E_b. \tag{16}$$

E_b is the polaron binding energy which is a sum of the interaction energies of the electron with the confined LO phonon in the well, the half-space LO phonon in the barrier material, and the IO phonon, respectively. It takes the form of

$$E_b = E_{LO1} + E_{LO2} + E_{IO}. \tag{17}$$

If we take $\hbar\omega_{L1}$ as the unit of energy, and the polaron radius R_p $(= (\hbar/2m_{b1}\omega_{L1})^{1/2})$ as the unit of length, then the expression can be given in a simple form.

(a) The interaction energy of the Q2D electron with the confined LO-phonon modes in the well material is given by

$$E_{LO1} = \frac{\alpha_1}{d}\sum_{m=1,2,3,\ldots}\frac{A_m}{1 + (B_m - 1)q_m^2}\ln(B_m + q_m^{-2}) \tag{18}$$

with

$$A_m = \frac{N_l d}{2}\left(1 + \frac{D_l}{k_l d}\frac{(m\pi)^2}{(m\pi)^2 - (2k_l d)^2}\right) \tag{19}$$

$$B_m = \frac{1 + (D_l/k_l d)\{1 - (2k_l d)^2/[(m\pi)^2 - (2k_l d)^2]\}}{1 + (D_l/k_l d)\{1 + (2k_l d)^2/[(m\pi)^2 - (2k_l d)^2]\}} \tag{20}$$

where $m \leqslant \mathrm{int}(W/a_0)$. a_0 and α_l are the lattice constant and the electron–LO-phonon coupling constant of the well material, respectively.

(b) The interaction energy of the electron with the half-space LO-phonon modes in the barrier materials is given by

$$E_{\mathrm{LO2}} = \alpha_2\left(\frac{\omega_{\mathrm{L2}}}{\omega_{\mathrm{L1}}}\right)^{3/2}\left(\frac{m_{\mathrm{b2}}}{m_{\mathrm{b1}}}\right)^{1/2}\frac{N_l C_l}{(V_l(V_0 - E_l))^{1/2}} \times\left\{1 - \left(\frac{V_0 - E_l}{V_l}\right)^{1/2}\ln\left[1 + \left(\frac{V_l}{V_0 - E_l}\right)^{1/2}\right]\right\} \tag{21}$$

with

$$V_l = \frac{\omega_{\mathrm{L2}}}{\omega_{\mathrm{L1}}}\frac{m_{\mathrm{b2}}}{m_{\mathrm{b1}}} + 2(V_0 - E_l) \tag{22}$$

where α_2 is the electron–LO-phonon coupling constant of the barrier material. ω_{L1} and ω_{L2} are the LO-phonon frequencies in the well and barrier materials, respectively.

(c) The interaction energy of the electron with the IO phonons has four terms correlated with the four branches of the IO phonon and is written as

$$E_{\mathrm{IO}} = \sum_{\sigma,p} E_{\mathrm{IO}}(\sigma, p) \tag{23}$$

where the index $p = +, -$ refers to the symmetric and antisymmetric IO-phonon modes, and $\sigma = +, -$ to the high- and low-frequency IO-phonon modes, respectively. The dispersion relation of the IO phonon with the (σ, p) indexes is given by the following equations:

$$\omega^2_{\pm p} = \frac{B_p(k) \pm \{B_p^2(k) - 4A_p(k)C_p(k)\}^{1/2}}{2A_p(k)} \tag{24}$$

where

$$A_p(k) = a_1^p + a_2^p \tag{25}$$

$$B_p(k) = a_1^p(\omega^2_{\mathrm{L1}} + \omega^2_{\mathrm{T2}}) + a_2^p(\omega^2_{\mathrm{L2}} + \omega^2_{\mathrm{T1}}) \tag{26}$$

$$C_p(k) = a_1^p\omega^2_{\mathrm{L1}}\omega^2_{\mathrm{T2}} + a_2^p\omega^2_{\mathrm{L2}}\omega^2_{\mathrm{T1}} \tag{27}$$

with

$$a_1^p = [1 - p\exp(-2kd)]\varepsilon_{\infty 1} \tag{28}$$

$$a_2^p = [1 + p\exp(-2kd)]\varepsilon_{\infty 2} \tag{29}$$

where $p = 1$ or $p = -1$ refers to $p = +$ or $p = -$.

The interaction energy of the electron with the branch of IO phonons specified by (σ, p) is given by

$$E_{IO}(\sigma, p) = 2\alpha_1 \bar{\varepsilon}_1 \int_0^\infty dk \frac{D^2_{\sigma p}(kd)}{\omega_{L1}\omega_{\sigma p}} [L_p(k) + F(k)]^2 \times \left[\left(\frac{\omega_{\sigma p}}{\omega_{L1}} + k^2 \right) L_p(k) + k^2 J_p(k) + \left(\frac{\omega_{\sigma p}}{\omega_{L1}} + 2\frac{m_{b2}}{m_{b1}} k^2 \right) F(k) \right]^{-1} \tag{30}$$

where

$$D_{\sigma p}(kd) = \{[1 + p\exp(-2kd)]/(2a_1^p \zeta_{1\sigma p} + 2a_2^p \zeta_{2\sigma p})\}^{1/2} \tag{31}$$

$$L_\pm(k) = \frac{S_\pm(k)}{\cosh(2kd) \pm 1} \tag{32}$$

$$J_\pm(k) = \frac{S_\mp(k)}{\cosh(2kd) \pm 1} \tag{33}$$

$$F(k) = N_l C_l \frac{1}{k_l' + k} \tag{34}$$

$$\bar{\varepsilon}_1 = (\varepsilon_{\infty 1}^{-1} - \varepsilon_{01}^{-1})^{-1} \tag{35}$$

with

$$S_\pm(k) = N_l \left[\frac{1}{k_l^2 + k^2} \sinh(2kd) \left(kC_l + \frac{k_l^2}{2k} \right) + \frac{k_l}{k_l^2 + k^2} D_l \cosh(2kd) \pm d \left(1 + \frac{D_l}{k_l d} \right) \right] \tag{36}$$

$$\zeta_{\lambda\sigma p} = \left(\frac{\omega_{L\lambda}^2 - \omega_{T\lambda}^2}{\omega_{T\lambda}^2 - \omega_{\sigma p}^2} \right)^2 \frac{\varepsilon_{\infty\lambda}}{\omega_{T\lambda}^2(\varepsilon_{0\lambda} - \varepsilon_{\infty\lambda})} \qquad (\lambda = 1, 2) \tag{37}$$

where ω_{T1} (ω_{T2}) is the transverse optical (TO) phonon frequency in the well (barrier) material.

Using the expressions above, one can easily calculate the energy spectrum and the individual contribution of every phonon mode to the polaronic correction. As far as we know, the present paper is the first work which gives the full energy spectrum of the Q2D electron–phonon interaction system in a QW structure. We feel that these expressions are useful for investigators working in this field.

Next, we apply equations (17)–(37) to the GaAs/$Ga_{1-x}Al_xAs$ QW to give some numerical results. The material parameters used in the calculation are the same as in [19] which are taken from [21]. Note that $Ga_{1-x}Al_xAs$ is a ternary mixed crystal; there exist two pairs of LO- and TO-phonon modes. In this paper we use the effective LO- and TO-phonon mode approximation [21]. Figure 1 shows the polaron binding energies in the lowest electronic subband state for $x = 0.3$ and 1.0 as functions of the well width. The contributions from the IO-, confined LO- and half-space LO-phonon modes are also shown as separate lines. Figure 2 gives the polaron binding energies for different electronic subband states with $x = 0.3$ and 1.0.

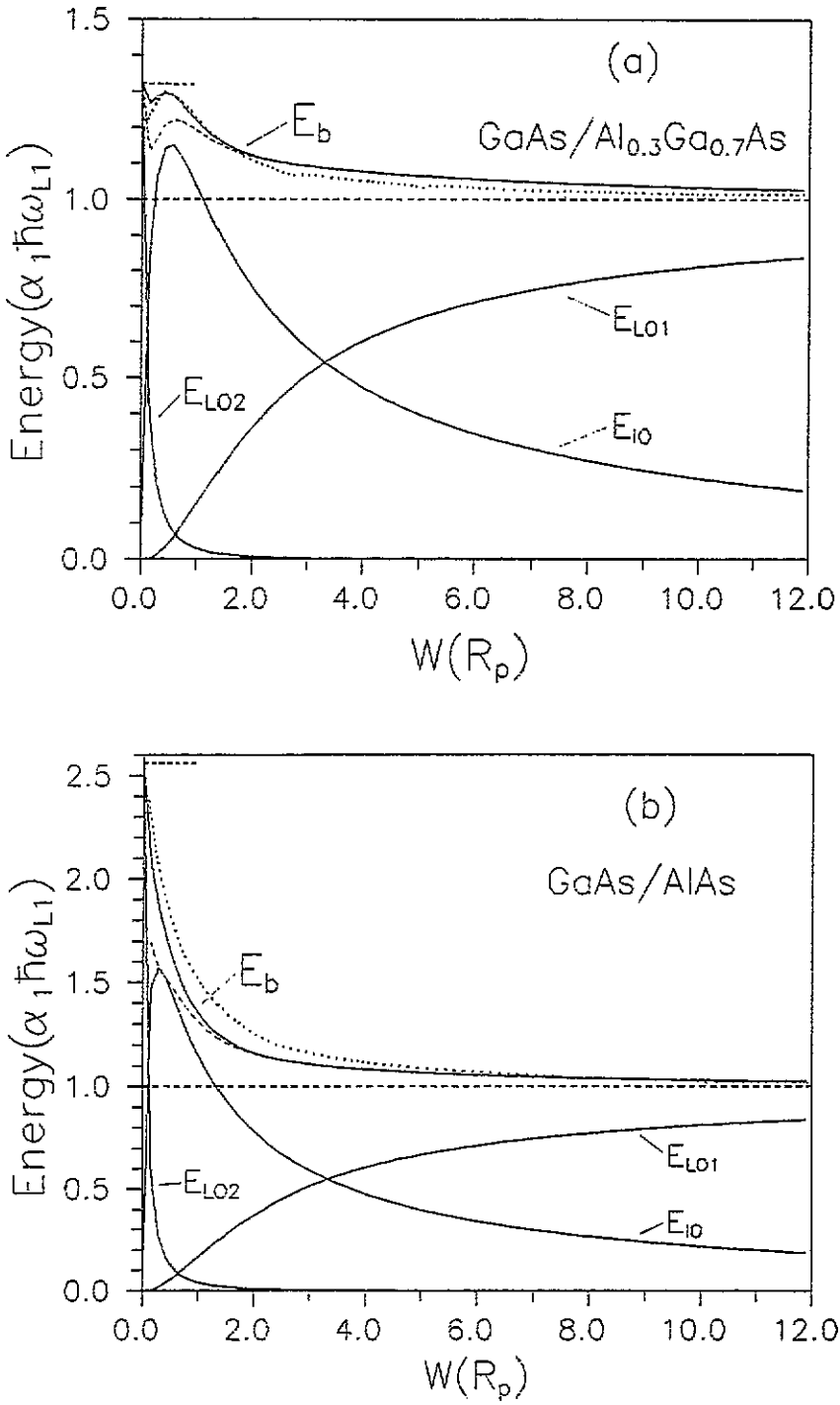

Figure 1. Polaron energy as a function of the well width W $(= 2d)$ in the GaAs/$Ga_{1-x}Al_xAs$ QW for different Al concentrations, where E_b represents the total binding energy of the Q2D polaron, and E_{LO1}, E_{LO2} and E_{IO} are the interaction energies of the confined electron with the confined LO-, half-space LO- and IO-phonons, respectively: ----, polaron binding energy obtained by the same-electron-band-mass approximation; ·····, polaron binding energy as given in [17].

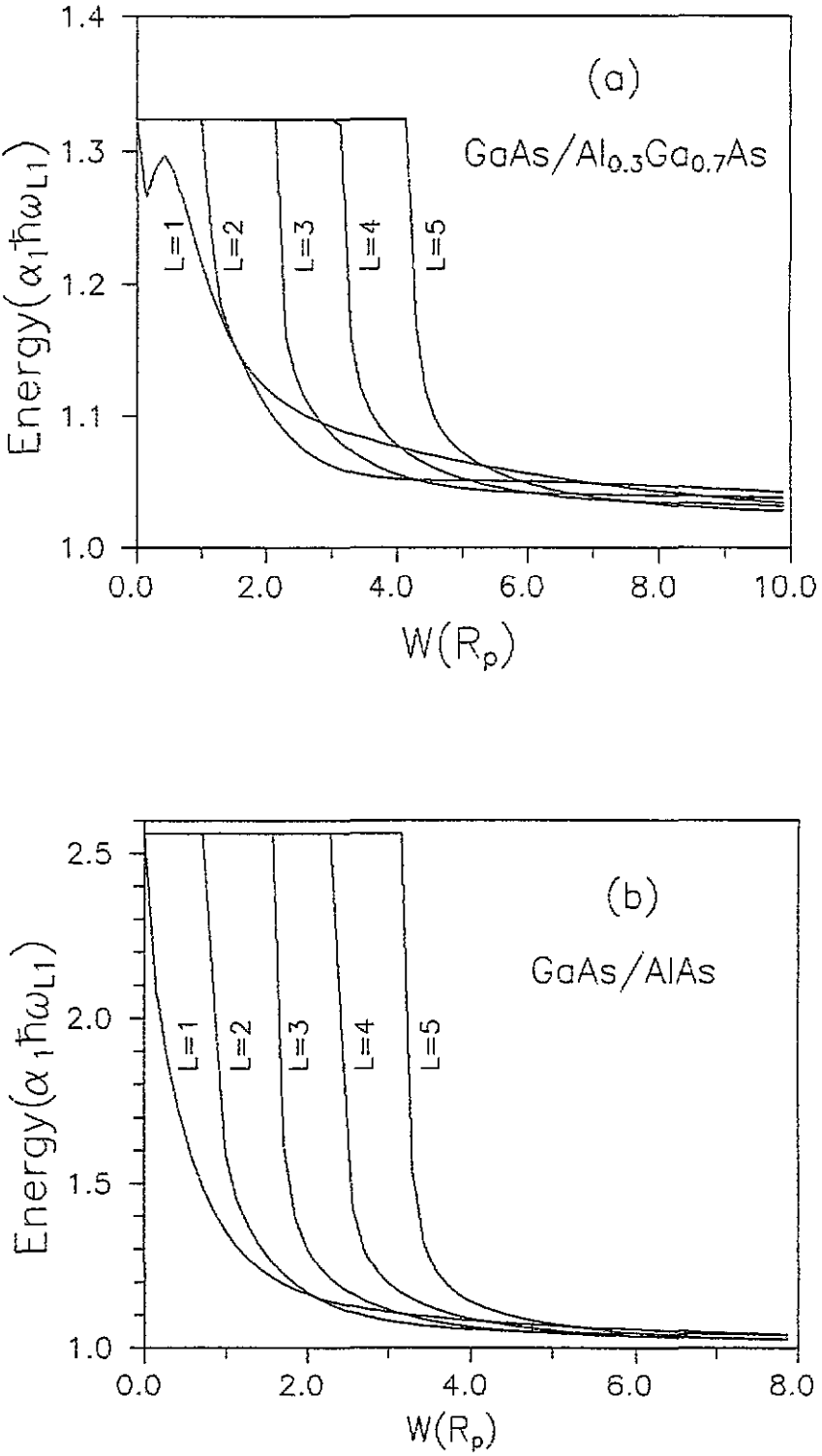

Figure 2. The total polaron binding energy at different electronic subband states as a function of the well width W $(= 2d)$ for different Al concentrations x in the GaAs/$Ga_{1-x}Al_xAs$ QW.

3. Discussion and conclusion

With a simple analytical calculation similar to [19], one can easily find that our theory gives correct limit results in the 2D and 3D limit cases, which can also be seen from figure 1 clearly. When the width of the QW is sufficiently large, the polaron binding energy reduces to $\alpha_1\hbar\omega_{L1}$ and, when the QW width decreases to zero, the polaron binding energy goes to $\alpha_2\hbar\omega_{L2}$. In the approximate cases, such as the infinite-height QW ($V_0 \to \infty$) or the same-electron-band-mass approximations ($m_{b1} = m_{b2} = m_b$), the expressions are reduced to those given in our previous papers [18, 19], respectively.

In figure 1, the broken curve represents the result with the approximation $m_{b1} = m_{b2}$, which was given in our previous paper [19]. As shown in figure 1, if the QW width is larger than about $2R_p$ the difference between the electron band masses in the well and barrier materials need not be considered but, when the well width is sufficiently narrow, the electron envelope function penetrates into the barrier material region obviously, and then the mass difference will have an obvious influence.

In order to compare the polaron binding energy given by the present variational method with that obtained by the perturbation method, we plot the numerical result taken from the paper of Hai *et al* [17] as a dotted curve in figure 1. One can see that the two results agree with each other, except for a little quantitative difference. After some analysis we think that this small difference may arise partly from the small fundamental differences between the Hamiltonians and parameters V_0 in the two studies. In the present paper, we use the expression proposed by Adachi [21] as the parameter V_0, which is

$$V_0 = \begin{cases} 1.1x & \text{for } 0 \leqslant x \leqslant 0.45 \\ 0.43 + 0.14x & \text{for } 0.45 < x \leqslant 1.0 \end{cases}$$

On the other hand, Hai *et al* used an empirical expression given by

$$V_0 = 0.6E_g = 0.6(1.155x + 0.37x^2).$$

We have noted that the binding energy obtained in the present variational calculation exhibits a minimum at a very narrow well width (about one or few monolayers) for the Al concentration $x < 0.5$. This feature was also found in [17]. It is caused by two competing effects, namely the drastic decrease in the contribution of the IO phonons and the drastic increase in the contribution of the LO phonons in the barrier materials as the well width decreases to zero. The sum of the two competing effects is sensitive to the selection of the calculation method and the parameters of the QW. Thus we feel that this minimum is only from the theoretical calculation and may not occur in a real sample of very narrow QW because the continuous model is invalid in this range.

From figure 2, one can see that, for the excited subband state, the polaron binding energy increases as the well width decreases up to the value of the free-bulk-polaron binding energy in the barrier material at a critical well width where the polaron state is really an extended state.

In conclusion, we have reported in the present paper a more advanced investigation on the properties of a Q2D polaron. A general analytical expression for the electron energy spectrum and the polaron binding energy for different electronic subband states of the Q2D electron–phonon interaction system is presented analytically. The expression is applied to $GaAs/Al_xGa_{1-x}As$ QWs numerically with several different aluminium concentrations x. The effects of the electronic subband state, the phonons and the confinement potential on the polaron corrections are shown clearly as the well width varies from infinity to zero.

Acknowledgment

This work is supported by the National Natural Science Foundation of China.

References

[1] Das Sarma S 1983 *Phys. Rev.* B 27 2590
[2] Das Sarma S and Stopa M 1987 *Phys. Rev.* B **36** 9595
[3] Degani M H and Hipólito O 1988 *Solid State Commun.* **65** 1185
[4] Wu Xiaoguang, Peeters F M and Devreese J T 1986 *Phys. Rev.* B **34** 2621, 8800
[5] Yildirim T and Ercelebi A 1991 *J. Phys.: Condens. Matter* **3** 1271, 4357
[6] Wendler L and Pechstedt R 1987 *Phys. Status Solidi* b **141** 129
[7] Tsuchiya T, Akera H and Ando T 1989 *Phys. Rev.* B **39** 6025
[8] Mori N and Ando T 1989 *Phys. Rev.* B **40** 6175
[9] Liang X X 1992 *J. Phys.: Condens. Matter* **4** 9769
[10] Liang X X and Davison S G 1993 *Surf. Sci.* **298** 225
[11] Chen R, Lin D L and George T F 1990 *Phys. Rev.* B **41** 1435
[12] Ridley B K and Babiker M 1991 *Phys. Rev.* B **43** 9096
[13] Ridley B K 1991 *Phys. Rev.* B **44** 9002
[14] Chamberlain M P, Cardona M and Ridley B K 1993 *Phys. Rev.* B **48** 14356
[15] Lin D L, Chen R and George T F 1991 *J. Phys.: Condens. Matter* **3** 4645
[16] Hai G Q, Peeters F M and Devreese J T 1990 *Phys. Rev.* B **42** 11063; 1993 *Phys. Rev.* B **47** 10358
[17] Hai G Q, Peeters F M and Devreese J T 1993 *Phys. Rev.* B **48** 4666
[18] Zheng R S, Ban S L and Liang X X 1994 *Phys. Rev.* B **49** 1796
[19] Zheng R S, Ban S L and Liang X X 1994 *Acta SNUN (China)* at press
[20] Bastard G 1981 *Phys. Rev.* B **24** 5693
[21] Adachi S 1985 *J. Appl. Phys.* **58** R1